Alexander Yu. Sokolov

Curriculum Vitae

(Last updated: May 22, 2024)

Contact Information

Address:	Department of Chemistry & Biochemistry The Ohio State University 2108 Newman & Wolfrom Laboratory 100 W. 18th Ave Columbus, OH 43210
Phone:	+1 (614) 688-3636
E-mail:	sokolov.8@osu.edu
Web:	http://research.cbc.osu.edu/sokolov.8/

Professional Experience

Current 5/2023	*Associate Professor* **The Ohio State University**, Columbus, OH (USA) Department of Chemistry & Biochemistry
8/2017 – 5/2023	*Assistant Professor* **The Ohio State University**, Columbus, OH (USA) Department of Chemistry & Biochemistry
7/2016 – 8/2017	*Postdoctoral Scholar* **California Institute of Technology**, Pasadena, CA (USA) Advisor: Professor Garnet K.-L. Chan
8/2014 – 6/2016	*Postdoctoral Research Associate* **Princeton University**, Princeton, NJ (USA) Advisor: Professor Garnet K.-L. Chan

Education

2009 – 2014	*Doctor of Philosophy* **University of Georgia**, Center for Computational Quantum Chemistry, Athens, GA (USA) Advisor: Professor Henry F. Schaefer III Thesis: "Development of density cumulant functional theory"
2004 – 2009	*Specialist Degree (M.S.)* **St. Petersburg State University**, St. Petersburg (Russia) *Diploma with Distinction* | Major: Chemistry Advisor: Professor Olga V. Sizova Thesis: "Valence structure analysis of heavy transition metal complexes with electronic configurations d^6, d^7, d^8, and d^{10}"

Academic Awards and Fellowships

2024	Dirac Medal from the World Association of Theoretical and Computational Chemists (WATOC)
2023	OpenEye Outstanding Junior Faculty Award in Computational Chemistry
2021	National Science Foundation CAREER Award
2016	American Chemical Society Physical Chemistry Division Postdoctoral Award
2015	IBM-Löwdin Award for Postdoctoral Associates, 55^{th} Sanibel Symposium, St. Simons' Island, GA (USA)
2014	Martin Reynolds Smith Award, University of Georgia, Athens, GA (USA)
2013	Dissertation Completion Award, University of Georgia, Athens, GA (USA)
2013	Best Graduate Student Poster Award, 53^{rd} Sanibel Symposium, St. Simons' Island, GA (USA)
2012	James L. Carmon Award, University of Georgia, Athens, GA (USA)
2009	Charles Coulson Fellowship, Center for Computational Quantum Chemistry, Athens, GA (USA), 5 years
2009	Best Alumnus of St. Petersburg 2009 Award, St. Petersburg (Russia)
2008	Special Scholarship of the Government of Russian Federation (Russia), 1 year
2008	Summer Fellowship, Center for Computational Quantum Chemistry, Athens, GA (USA)
2004	Full Scholarship, St. Petersburg State University (Russia), 5 years

Publications (h-index: 19)

* *Corresponding authors are denoted with asterisk.*

[52] T. L. Stahl and **A. Yu. Sokolov***. "Quantifying spin contamination in algebraic diagrammatic construction theory of electronic excitations." *J. Chem. Phys.* **160**, 204104 (2024).

[51] N. E. Sparks, C. Smith, T. Stahl, D. L. Amarasekara, C. Hamadani, E. Lambert, S. W. Tang, A. Kulkarni, B. M. Derbigny, G. S. Dasanayake, G. Taylor, M. Ghazala, N. I. Hammer, **A. Yu. Sokolov**, N. C. Fitzkee, E. E. L. Tanner, and D. L. Watkins*. "NIR-II emissive donor–acceptor–donor fluorophores for dual fluorescence bioimaging and photothermal therapy applications." *J. Mat. Chem. C* **12**, 4369–4383 (2024).

[50] S. Carter, W. Tao, R. Majumder, **A. Yu. Sokolov***, and S. Zhang. "Two-State Hydrogen Atom Transfer Reactivity of Unsymmetric $[Cu_2(O)(NO)]^{2+}$ Complexes." *J. Am. Chem. Soc.* **145**, 17779–17785 (2023).

[49] I. M. Mazin and **A. Yu. Sokolov***. "Core-Excited States and X-ray Absorption Spectra from Multireference Algebraic Diagrammatic Construction Theory." *J. Chem. Theory Comput.* **19**, 4991–5006 (2023).

[48] S. Banerjee and **A. Yu. Sokolov***. "Algebraic Diagrammatic Construction Theory for Simulating Charged Excited States and Photoelectron Spectra." *J. Chem. Theory Comput.* **19**, 3037–3053 (2023). (**Highlight: invited review**).

[47] S. Bandaranayake, A. Patnaik, E. Hruska, Q. Zhu, **A. Yu. Sokolov**, and L. R. Baker*. "Electronic Structure and Ultrafast Electron Dynamics in CuO Photocatalysts Probed by Surface Sensitive Femtosecond X-ray Absorption Near-Edge Structure Spectroscopy." *J. Phys. Chem. Lett.* **14**, 3643–3650 (2023).

[46] J. K. Bower, M. S. Reese, I. M. Mazin, L. M. Zarnitsa, A. D. Cypcar, C. E. Moore, **A. Yu. Sokolov***, and S. Zhang*. "C(sp^3)–H cyanation by a formal copper(iii) cyanide complex." *Chem. Sci.* (2023).

[45] R. Majumder and **A. Yu. Sokolov***. "Simulating Spin–Orbit Coupling with Quasidegenerate N-Electron Valence Perturbation Theory." *J. Phys. Chem. A* **127**, 546–559 (2023). (**Highlight: invited article, "Early-Career and Emerging Researchers in Physical Chemistry" special issue**).

[44] S. Lin, S. Banerjee, M. T. Fortunato, C. Xue, J. Huang, **A. Yu. Sokolov***, and C. Turro*. "Electrochemical Strategy for Proton Relay Installation Enhances the Activity of a Hydrogen Evolution Electrocatalyst." *J. Am. Chem. Soc.* **144**, 20267–20277 (2022).

[43] S. Banerjee and **A. Yu. Sokolov***. "Non-Dyson Algebraic Diagrammatic Construction Theory for Charged Excitations in Solids." *J. Chem. Theory Comput.* **18**, 5337–5348 (2022).

[42] T. L. Stahl, S. Banerjee, and **A. Yu. Sokolov***. "Quantifying and reducing spin contamination in algebraic diagrammatic construction theory of charged excitations." *J. Chem. Phys.* **157**, 044106 (2022).

[41] C. E. V. de Moura and **A. Yu. Sokolov***. "Simulating X-ray photoelectron spectra with strong electron correlation using multireference algebraic diagrammatic construction theory." *Phys. Chem. Chem. Phys.* **24**, 4769–4784 (2022). (**Highlight: PCCP HOT Article**).

[40] I. M. Mazin and **A. Yu. Sokolov***. "Multireference Algebraic Diagrammatic Construction Theory for Excited States: Extended Second-Order Implementation and Benchmark." *J. Chem. Theory Comput.* **17**, 6152–6165 (2021).

[39] S. Banerjee and **A. Yu. Sokolov***. "Efficient implementation of the single-reference algebraic diagrammatic construction theory for charged excitations: Applications to the TEMPO radical and DNA base pairs." *J. Chem. Phys.* **154**, 074105 (2021). (**Highlight: Invited article, 2021 JCP Emerging Investigators Special Collection**).

[38] J. P. Misiewicz, J. M. Turney, H. F. Schaefer*, and **A. Yu. Sokolov**. "Assessing the orbital-optimized unitary Ansatz for density cumulant theory." *J. Chem. Phys.* **153**, 244102 (2020).

[37] K. Chatterjee and **A. Yu. Sokolov***. "Extended Second-Order Multireference Algebraic Diagrammatic Construction Theory for Charged Excitations." *J. Chem. Theory Comput.* **16**, 6343–6357 (2020).

[36] Q. Sun, X. Zhang, S. Banerjee, P. Bao, M. Barbry, N. S. Blunt, N. A. Bogdanov, G. H. Booth, J. Chen, Z.-H. Cui, J. J. Eriksen, Y. Gao, S. Guo, J. Hermann, M. R. Hermes, K. Koh, P. Koval, S. Lehtola, Z. Li, J. Liu, N. Mardirossian, J. D. McClain, M. Motta, B. Mussard, H. Q. Pham, A. Pulkin, W. Purwanto, P. J. Robinson, E. Ronca, E. R. Sayfutyarova, M. Scheurer,

H. F. Schurkus, J. E. T. Smith, C. Sun, S.-N. Sun, S. Upadhyay, L. K. Wagner, X. Wang, A. F. White, J. D. Whitfield, M. J. Williamson, S. Wouters, J. Yang, J. M. Yu, T. Zhu, T. C. Berkelbach, S. Sharma, **A. Yu. Sokolov**, and G. K.-L. Chan*. "Recent developments in the PySCF program package." *J. Chem. Phys.* **153**, 024109 (2020).

[35] D. G. A. Smith, L. A. Burns, A. C. Simmonett, R. M. Parrish, M. C. Schieber, R. Galvelis, P. Kraus, H. Kruse, R. Di Remigio, A. Alenaizan, A. M. James, S. Lehtola, J. P. Misiewicz, M. Scheurer, R. A. Shaw, J. B. Schriber, Y. Xie, Z. L. Glick, D. A. Sirianni, J. S. O'Brien, J. M. Waldrop, A. Kumar, E. G. Hohenstein, B. P. Pritchard, B. R. Brooks, H. F. Schaefer, **A. Yu. Sokolov**, K. Patkowski, A. E. DePrince III, U. Bozkaya, R. A. King, F. A. Evangelista, J. M. Turney, T. D. Crawford, and C. D. Sherrill*. "PSI4 1.4: Open-source software for high-throughput quantum chemistry." *J. Chem. Phys.* **152**, 184108 (2020).

[34] S. Banerjee and **A. Yu. Sokolov***. "Third-order algebraic diagrammatic construction theory for electron attachment and ionization energies: Conventional and Green's function implementation." *J. Chem. Phys.* **151**, 224112 (2019).

[33] K. Chatterjee and **A. Yu. Sokolov***. "Second-order multireference algebraic diagrammatic construction theory for photoelectron spectra of strongly correlated systems." *J. Chem. Theory Comput.* **15**, 5908–5924 (2019).

[32] J. K. Bower, **A. Yu. Sokolov**, and S. Zhang*. "Four-coordinate copper halonitrosyl $(CuNO)^{10}$ complexes." *Angew. Chem. Int. Ed.* **58**, 10225–10229 (2019).

[31] R. Peng, A. V. Copan, and **A. Yu. Sokolov***. "Simulating X-ray absorption spectra with linear-response density cumulant theory." *J. Phys. Chem. A* **123**, 1840–1850 (2019). (**Highlight: Invited article, "Young Scientists" virtual special issue**).

[30] **A. Yu. Sokolov***. "Multi-reference algebraic diagrammatic construction theory for excited states: General formulation and first-order implementation." *J. Chem. Phys.* **149**, 204113 (2018). (**Highlight: JCP Editors' Pick article**).

[29] A. V. Copan and **A. Yu. Sokolov***. "Linear-response density cumulant theory for excited electronic states." *J. Chem. Theory Comput.* **14**, 4097–4108 (2018).

[28] R. M. Parrish, L. A. Burns, D. G. A. Smith, A. C. Simmonett, A. E. DePrince, E. G. Hohenstein, U. Bozkaya, **A. Yu. Sokolov**, R. Di Remigio, R. M. Richard, J. F. Gonthier, A. M. James, H. R. McAlexander, A. Kumar, M. Saitow, X. Wang, B. P. Pritchard, P. Verma, H. F. Schaefer, K. Patkowski, R. A. King, E. F. Valeev, F. A. Evangelista, J. M. Turney, T. D. Crawford, and C. D. Sherrill*. "Psi4 1.1: An open-source electronic structure program emphasizing automation, advanced libraries, and interoperability." *J. Chem. Theory Comput.* **13**, 3185–3197 (2017).

[27] **A. Yu. Sokolov***, S. Guo, E. Ronca, and G. K.-L. Chan*. "Time-dependent N-electron valence perturbation theory with matrix product state reference wavefunctions for large active spaces and basis sets: Applications to the chromium dimer and all-trans polyenes." *J. Chem. Phys.* **146**, 244102 (2017).

[26] X. Wang, **A. Yu. Sokolov***, J. M. Turney, and H. F. Schaefer*. "Spin-adapted formulation and implementation of density cumulant functional theory with density-fitting approximation: Application to transition metal compounds." *J. Chem. Theory Comput.* **12**, 4833–4842 (2016).

[25] **A. Yu. Sokolov*** and G. K.-L. Chan*. "A time-dependent formulation of multi-reference perturbation theory." *J. Chem. Phys.* **144**, 064102 (2016). (**Highlight: JCP 2016 Editors' Choice article**).

[24] J. W. Mullinax, **A. Yu. Sokolov**, and H. F. Schaefer*. "Can density cumulant functional theory describe static correlation effects?" *J. Chem. Theory Comput.* **11**, 2487–2495 (2015).

[23] **A. Yu. Sokolov*** and G. K.-L. Chan*. "A transformed framework for dynamic correlation in multireference problems." *J. Chem. Phys.* **142**, 124107 (2015).

[22] **A. Yu. Sokolov***, H. F. Schaefer, and W. Kutzelnigg. "Density cumulant functional theory from a unitary transformation: N-representability, three-particle correlation effects, and application to O_4^+." *J. Chem. Phys.* **141**, 074111 (2014).

[21] J. W. Mullinax*, **A. Yu. Sokolov**, and H. F. Schaefer. "Conical intersections and low-lying electronic states of tetrafluoroethylene." *ChemPhysChem* **15**, 2359–2366 (2014).

[20] A. V. Copan*, **A. Yu. Sokolov**, and H. F. Schaefer. "Benchmark study of density cumulant functional theory: thermochemistry and kinetics." *J. Chem. Theory Comput.* **10**, 2389–2398 (2014).

[19] **A. Yu. Sokolov*** and H. F. Schaefer. "Orbital-optimized density cumulant functional theory." *J. Chem. Phys.* **139**, 204110 (2013).

[18] **A. Yu. Sokolov***, D. B. Magers, J. I. Wu, W. D. Allen*, P. v. R. Schleyer, and H. F. Schaefer. "Free cyclooctatetraene dianion: planarity, aromaticity, and theoretical challenges." *J. Chem. Theory Comput.* **9**, 4436–4443 (2013).

[17] Y. Qiu, **A. Yu. Sokolov**, Y. Yamaguchi, and H. F. Schaefer*. "$BeCH_2$: the simplest metal carbene. High levels of theory." *J. Phys. Chem. A* **117**, 9266–9273 (2013).

[16] S. Vogt-Geisse, **A. Yu. Sokolov**, S. R. McNew, Y. Yamaguchi, and H. F. Schaefer*. "Structures and transition states of Ge_2CH_2." *J. Phys. Chem. A* **117**, 5765–5774 (2013).

[15] **A. Yu. Sokolov***, A. C. Simmonett, and H. F. Schaefer. "Density cumulant functional theory: the DC-12 method, an improved description of the one-particle density matrix." *J. Chem. Phys.* **138**, 024107 (2013).

[14] **A. Yu. Sokolov***, S. Mittal, A. C. Simmonett, and H. F. Schaefer III. "Characterization of the t-butyl radical and its elusive anion." *J. Chem. Theory Comput.* **8**, 4323–4329 (2012).

[13] **A. Yu. Sokolov***, J. J. Wilke, A. C. Simmonett, and H. F. Schaefer III. "Analytic gradients for density cumulant functional theory: the DCFT-06 model." *J. Chem. Phys.* **137**, 054105 (2012).

[12] **A. Yu. Sokolov*** and H. F. Schaefer III. "Ground and excited state properties of photoactive platinum(IV) diazido complexes: theoretical considerations." *Dalton Trans.* **40**, 7571–7582 (2011).

[11] **A. Yu. Sokolov*** and H. F. Schaefer III. "Coordination properties of bridging diazene ligands in unusual diiron complexes." *Organometallics* **29**, 3271–3280 (2010).

[10] **A. Yu. Sokolov** and O. V. Sizova*. "Quantum-chemical study of trans-influence in gold(I) linear complexes." *Russ. J. Gen. Chem.* **80**, 1223–1231 (2010).

[9] V. V. Pakal'nis*, **A. Yu. Sokolov**, A. A. Slisenko, M. E. Borovitov, S. P. Tunik, and O. V. Sizova. "Synthesis and spectral characteristics of a novel heterometallic binuclear complex on the basis of 3,6-bis(2-pyridyl)-1,2,4,5-tetrazine." *Russ. J. Gen. Chem.* **79**, 980–984 (2009).

[8] O. V. Sizova*, L. V. Skripnikov, **A. Yu. Sokolov**, and V. V. Sizov. "Atomic-orbital-symmetry based σ-, π-, and δ-decomposition analysis of bond orders." *Int. J. Quant. Chem.* **109**, 2581–2590 (2009).

[7] O. V. Sizova*, L. V. Skripnikov, and **A. Yu. Sokolov**. "Calculation of σ-, π-, and δ-components of quantum-chemical bond orders." *Russ. J. Gen. Chem.* **78**, 2146–2147 (2008).

[6] O. V. Sizova*, L. V. Skripnikov, and **A. Yu. Sokolov**. "Symmetry decomposition of quantum-chemical bond orders." *J. Mol. Struct. (THEOCHEM)* **870**, 1–9 (2008).

[5] **A. Yu. Sokolov**, N. J. Stibrich, and H. F. Schaefer* III. "BO_3 molecular structures: examples of the importance of electron correlation." *Coll. Czech. Chem. Commun.* **73**, 1495–1508 (2008).

[4] O. V. Sizova*, **A. Yu. Sokolov**, and L. V. Skripnikov. "Quantum-chemical study of donor-acceptor interactions in chelate dicarbonyl complexes of rhodium(I)." *Russ. J. Coord. Chem.* **33**, 800–808 (2007).

[3] O. V. Sizova*, **A. Yu. Sokolov**, L. V. Skripnikov, and V. I. Baranovski. "Quantum chemical study of the bond orders in the ruthenium, diruthenium and dirhodium nitrosyl complexes." *Polyhedron* **26**, 4680–4690 (2007).

[2] O. V. Sizova*, L. V. Skripnikov, **A. Yu. Sokolov**, and N. V. Ivanova. "Rhodium and ruthenium tetracarboxylate nitrosyl complexes: electronic structure and metal-metal bond." *Russ. J. Coord. Chem.* **33**, 588–593 (2007).

[1] O. V. Sizova*, L. V. Skripnikov, **A. Yu. Sokolov**, and O. O. Lyubimova. "Features of the electronic structure of ruthenium tetracarboxylates with axially coordinated nitric oxide (II)." *J. Struct. Chem.* **48**, 28–36 (2007).

Invited Conference Presentations

06/2025	WATOC 2025 Congress, Oslo (Norway)
06/2023	Conference "Quantum International Frontiers", Lodz (Poland)
06/2023	Symposium "Advances in Theoretical and Computational Chemistry", Vancouver (Canada)
04/2023	Workshop on Excited-State Methodologies, Toulouse (France)
03/2023	COMP Awards Symposium, ACS National Meeting, Indianapolis, IN (USA)
06/2022	10^{th} Molecular Quantum Mechanics (MQM) Congress, Blacksburg, VA (USA)
06/2022	International Workshop on Reduced Density Matrix Theory for Quantum Many-Fermion Systems, San Sebastian (Spain)
02/2022	Sanibel Symposium, St. Simon's Island, GA (USA)
12/2021	Symposium "Computational Quantum Chemistry: Synergism Between Theory and Experiment" (virtual), Pacifichem 2020, Honolulu, HI (USA)

07/2021	Workshop "New Developments in Coupled-Cluster Theory" (virtual), Telluride, CO (USA)
06/2021	Conference "New Frontiers in Electron Correlation" (virtual), Telluride, CO (USA)
06/2020	Conference "Low-scaling and Unconventional Electronic Structure Techniques" (LUEST) (virtual), Telluride, CO (USA)
08/2019	Symposium "Computational Quantum Chemistry: From Promise to Prominence", 258^{th} ACS National Meeting, San Diego, CA (USA)
07/2019	32^{nd} Midwest Undergraduate Computational Chemistry Consortium Conference, Columbus, OH (USA)
06/2019	Workshop "Fundamental Challenges of Electron-Density-Based Approaches to Time-Dependent Processes and Open Quantum Systems", ETH Zürich (Switzerland)
03/2019	Symposium "Quantum Mechanics: Strong Correlation", 257^{th} ACS National Meeting, Orlando, FL (USA)
11/2018	Psi4 Annual Developer's Conference (PsiCon), Atlanta, GA (USA)
06/2018	50^{th} Midwest Theoretical Chemistry Conference, Chicago, IL (USA)
08/2017	Workshop "New Developments in Coupled-Cluster Theory", Telluride, CO (USA)
05/2017	Symposium "Electronic Structure Theory", 100^{th} Canadian Chemistry Conference, Toronto (Canada)
04/2017	Symposium "Strong Electron Correlation & Nonadiabatic Dynamics", 253^{rd} ACS National Meeting, San Francisco, CA (USA)
08/2016	Symposium "Metal & Semiconductor Nanoclusters with Atomic Precision: Fundamentals & Applications", *ACS Physical Chemistry Division Postdoctoral Award Talk*, 252^{nd} ACS National Meeting, Philadelphia, PA (USA)
06/2016	8^{th} Molecular Quantum Mechanics (MQM) Congress, Uppsala University, Uppsala (Sweden)
03/2016	Symposium "Towards Predictive Calculations in Strongly Correlated Molecules and Materials", 251^{st} ACS National Meeting, San Diego, CA (USA)
08/2015	Workshop on Quantum Marginals and Numerical Ranges, University of Guelph, Guelph (Canada)
05/2014	Annual Meeting of the Southeast Theoretical Chemistry Association (SETCA 2014), Atlanta, GA (USA)
09/2013	Quantum Mechanics in Many Dimensions, 246^{th} ACS National Meeting, Indianapolis, IN (USA)

Invited Seminars

01/2024 | Heidelberg University, Heidelberg (Germany)

10/2023 | Akron University, Akron, OH (USA)

10/2022 | John's Hopkins University, Baltimore, MD (USA)

10/2022 | Northeastern University, Boston, MA (USA)

04/2022 | Emory University, Atlanta, GA (USA)

04/2022 | University of Michigan, Ann Arbor, MI (USA)

04/2022 | University of Washington, Seattle, WA (USA)

03/2022 | University of California, Berkeley, CA (USA)

02/2022 | University of Florida, Gainesville, FL (USA)

02/2022 | Florida State University, Tallahassee, FL (USA)

01/2022 | University of Chicago, Chicago, IL (USA)

Students and Postdocs Supervised

Graduate students:

- Nicholas Chiang (2023 – present)
- James Serna (2023 – present)
- Donna Odhiambo (2022 – present)
- Abdelrahman Ahmed (2020 – present)
- Rajat Majumder (2019 – present)
- Terrence Stahl (Ph.D., 2024)
- Ilia Mazin (Ph.D., 2023)
- Samragni Banerjee (Ph.D., 2022)

Undergraduate students:

- Bryce Pickett (2023 – present)
- Guowei (Peter) Qu (2022 – present)
- Mallard Woodward (B.S., 2024)
- Yichen Fan (B.S., 2021)
- Ruojing Peng (B.S., 2019)

Postdocs:

- Carlos Eduardo Vieira de Moura (2021 – 2023)
- Koushik Chatterjee (2018 – 2020)

Teaching Experience

Since 2023	Quantum Mechanics and Spectroscopy (CHEM 6510), *Instructor*, OSU
Since 2019	Physical Chemistry I (CHEM 4300), *Instructor*, OSU
2018 – 2021	Advanced Quantum Mechanics and Spectroscopy (CHEM 7520), *Instructor*, OSU
2011 – 2014	Advanced Quantum Chemistry (CHEM 8950), *Teaching Assistant*, UGA
2011, 2012	Summer Undergraduate Fellowship Program, *Instructor and Mentor*, Center for Computational Quantum Chemistry, UGA

Professional Service (External)

- Co-organizer, National ACS Meeting Symposium "Quantum Chemistry: Current and Future Frontiers", Chicago, IL, USA (08/2022)
- Co-organizer, Midwest Theoretical Chemistry Conference, Columbus, OH, USA (06/2022)
- Reviewer for the funding agencies and computing facilities (2017 – present): National Science Foundation, Department of Energy, American Chemical Society Petroleum Research Fund, German Research Foundation, Swiss National Science Foundation, The Ohio Supercomputer Center
- Reviewer for the scientific journals (2014 – present): Journal of Chemical Theory and Computation, Journal of Chemical Physics, Journal of American Chemical Society, Journal of Physical Chemistry Letters, Journal of Physical Chemistry A, Physical Chemistry Chemical Physics, Dalton Transactions, International Journal of Quantum Chemistry, WIREs Computational Molecular Science, Theoretical Chemistry Accounts, New Journal of Chemistry, Acta Physica Polonica A

Professional Service (OSU)

- Center for Quantum Information Science and Engineering Advisory Board (2022 – present)
- Coordinator, Physical Chemistry Seminar Series (2020 – present)
- Graduate Student Admissions Committee (2019 – present)
- Physical Division Faculty Search Committee (2023 – 2024)
- Temporary Advisor for the First-Year Graduate Students (2020 – 2022)
- Graduate Student Recruitment Committee (2018 – 2019)

Professional Organizations

- Member, Center for Quantum Information Science and Engineering (since 2022)
- Member, PySCF Board of Directors (since 2019)
- Member, Institute for Optical Science, OSU, Columbus, OH, USA (since 2019)
- Member of the COMP and PHYS divisions of American Chemical Society (since 2012, member # 30196915)

Research Funding

- "Flexible Embedding Framework for Efficient and Accurate Spectroscopic Simulations of Crystalline Defects With Applications in Quantum Science", NMS Exploratory Grant Program, $48,000 (1/2024 – 12/2024).
- "Efficient and Reliable Electronic Structure Theories for Spectroscopic Properties of Strongly Correlated Systems", National Science Foundation CAREER Award, $650,000 (5/2021 – 4/2026).
- "Elucidating Spectroscopic Properties of Heterogeneous Transition Metal Oxide Catalysts with Accurate Electronic Structure Theory", American Chemical Society Petroleum Research Fund, $110,000 (9/2022 – 8/2024).
- "Creating quantum bits based on rare-earth ions for quantum networking", The Ohio State University President's Research Excellence Program, $200,000, (1/2022 – 12/2023). Co-PI with Ronald M. Reano, Daniel Gauthier, Ezekiel Johnston–Halperin, Roland Kawakami, Gregory Lafyatis.